Estimation of Binary Infinite Dilute Diffusion Coefficient Using Artificial Neural Network

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(Received 6 August 2013, Accepted 29 October 2013)

Abstract

In this study, the use of the three-layer feed forward neural network has been investigated for estimating of infinite dilute diffusion coefficient (D_{12}) of supercritical fluid (SCF), liquid and gas binary systems. Infinite dilute diffusion coefficient was spotted as a function of critical temperature, critical pressure, critical volume, normal boiling point, molecular volume in normal boiling point, molecule diameter, Lennard-Jones's (LJ) energy parameter, temperature and pressure. For each set of SCF, liquid and gas systems a three-layer network has been applied with training algorithm of Levenberg-Marquard (LM). The obtained results of models have shown good accuracy of artificial neural network (ANN) for estimating infinite dilute diffusion coefficient of SCF, liquid and gas binary systems with mean relative error (MRE) of 2.88 % for 231 systems containing 4078 data points (mean relative error for ANN model in SCF, liquid and gas binary systems are 3.00, 2.99 and 1.21 %, respectively).

Keywords: Artificial neural network, Binary mixture, Infinite dilute diffusion coefficient, Supercritical fluid

Introduction

Infinite dilute diffusion coefficient (D_{12}) is one of the most important transport properties. In which molecule 1 is solvent and molecule 2 is solute, which each molecule 2 is in an environment of pure molecule 1. Concentration of molecule 2 is up to 5 and perhaps 10 mole percent [1]. In some of the industrial processes such as extraction from SCFs, mixing of concentrated liquids and gas systems in low densities, systems can be supposed as infinite dilute condition. For this reason numerous equations have been presented for estimating this property. These equations are on the base of ideal gas, Enskog fluid, hard sphere fluid, LJ fluid and real fluid theories [2].

Although different theories and semi-empirical correlations has been offered for estimating of infinite dilute diffusion coefficient, remarkable difference are observed between results and real values. In addition, each correlation has a high accuracy only for special group of fluids. Since last two decade using of neural network has a wide spread application to solve different problems of chemical engineering [3-15]. Recently Eslamloueyan and Khademi [15] were investigated a three-layer feed forward neural network to estimate gases binary diffusion coefficient in atmospheric pressure. In their suggested model, temperature, critical temperature, critical volume and molecular weight are spotted as input data of the network.

In this work, three-layer feed forward neural network was used for estimating infinite dilute diffusion coefficient of binary SCF, liquid and gas systems separately. Results were shown good accuracy of models in comparison with experimental data and the other models.

1. Methodology

Natural ability of artificial neural network can be used for learning and recognizing of non-linear and complex correlation, to estimate infinite dilute diffusion coefficient of SCF, liquid and gas systems. A briefly review on ANN that was used in this study, has been done by Eslamloueyan and Khademi [13].

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1.1. Analyzing and using of data

In this work a large complex of data were compiled that consists of 231 systems and 4078 data points (binary mixtures of SCF (111 systems/3277 points), binary liquid (88 systems/549 points) and binary gas mixtures (32 systems/252 points)). An ANN was used for each one of SCF, liquid and gas systems. Table 1 shows the studied systems, number of data point (NDP) and sources of data. Three-fourths of data were used for training of network and the rest used for test. In these models infinite dilute diffusion coefficient is spotted as a function of molecular weight, critical properties, normal boiling point, molar volume in normal boiling point, molecule diameter, LJ energy parameter, temperature and pressure:

$$D_{12} = f\begin{pmatrix} M_1, T_{c1}, P_{c1}, V_{c1}, T_{bp1}, V_{bp1}, \sigma_{LJ1}, \\ \{\varepsilon_{LJ} / k_B\}_1, M_2, T_{c2}, P_{c2}, V_{c2}, \\ T_{bp2}, V_{bp2}, \sigma_{LJ2}, \{\varepsilon_{LJ} / k_B\}_2, T, P \end{pmatrix} \quad (1)$$

Table 1: Studied systems and data sources

System		NDP	Data sources
Solvent (1)	**Solute (2)**		
	Supercritical systems		
2,3-Dimethylbutane	Benzene	11	[16]
	Napthalene	9	[16]
	Phenanthrene	11	[16]
	Toluene	10	[16]
Carbon dioxide	1,3-Divinylbenzene	15	[17]
	2,3-Dimethylaniline	15	[18]
	2,6-Dimethylaniline	15	[18]
	2-Bromoanisole	15	[17]
	2-Fluoroanisole	15	[17]
	2-Methylanisole	15	[18]
	3-Nitrotoluene	15	[18]
	4-Methylanisole	15	[18]
	Allylbenzene	15	[17]
	γ-Linolenic acid	142	[19]
	γ-Linolenic acid ethyl ester	44	[19]
	γ-Linolenic acid methyl ester	55	[19, 20]
	1,1,1,5,5,5-Hexafluoroacetylacetone	15	[21]
	1,2-Dichlorobenzene	15	[22]
	1,2-Diethylbenzene	15	[23]
	1,3,5-Trimethylbenzene	22	[24, 25]
	15-Crown-5	30	[26]
	1-Phenyldodecane	15	[27]
	1-Phenylethanol	15	[28]
	1-Phenylhexane	15	[27]
	1-Phenyloctane	15	[27]
	1-Propanol	17	[29]

Table 1: Continued

System		NDP	Data sources
Solvent (1)	**Solute (2)**		
Supercritical systems			
Carbon dioxide	2,4-Dimethylphenol	15	[30]
	2-Butanone	38	[31]
	2-Ethyltoluene	15	[32]
	2-Pentanone	24	[31]
	2-Phenyl-1-propanol	15	[28]
	2-Phenylethanol	15	[28]
	2-Phenylethyl acetate	15	[33]
	3-Pentanone	39	[31]
	3-Phenyl-1-propanol	15	[28]
	3-Phenylpropyl acetate	15	[33]
	α–Linolenic acid	56	[34]
	AA ethyl ester	48	[35]
	Acetone	184	[24, 31, 36, 37]
	Acridine	6	[38]
	Aniline	15	[25]
	Anisole	15	[30]
	α–Pinene	15	[39]
	Arachidonic acid (AA)	75	[40]
	α–Tocopherol	82	[41-43]
	β–Carotene	90	[41-43]
	Behenic acid ethyl ester	34	[44, 45]
	Benzene	249	[24, 46-50]
	Benzoic acid	32	[29, 38, 51]
	Benzyl acetate	15	[33]
	Benzylacetone	15	[52]
	Biphenyl	27	[51]
	Bromobenzene	15	[53]
	Butyric acid ethyl ester	16	[45]
	Caffeine	21	[54]
	Capric acid ethyl ester	16	[45]
	Caprylic acid ethyl ester	16	[45]
	Chlorobenzene	15	[53]
	Chrysene	4	[24]
	Citral	15	[55]
	Cobalt(III) acetylacetonate	38	[56]
	Copper(II) Trifluoroacetylacetonate	12	[21]
	DHA ethyl ester	17	[44]
	DHA methyl ester	17	[44]
	Dibenzo-24-crown-8	28	[26]
	Dibenzyl ether	15	[33]
	Diethyl ether	15	[57]
	Diisopropyl ether	15	[57]
	Diolein	9	[58]
	d-limonene	15	[55]
	Docosahexaenoic acid (DHA)	80	[34, 45]
	Eicosapentaenoic acid (EPA)	72	[34, 45]

Table 1: Continued

System		NDP	Data sources
Solvent (1)	**Solute (2)**		
Supercritical systems			
Carbon dioxide	EPA methyl ester	17	[44]
	Ethanol	24	[29]
	Ethyl acetate	15	[54]
	Ethyl benzoate	15	[52]
	Eugenol	15	[52]
	Fluorobenzene	15	[53]
	Hexachlorobenzene	13	[59]
	Iodobenzene	15	[53]
	Linalool	15	[46]
	Linoleic acid	71	[40]
	Methanol	10	[29]
	Monoolein	11	[58]
	Myristic acid ethyl ester	16	[45]
	Naphthalene	41	[24, 59, 60]
	n-Butylbenzene	15	[27]
	Nitrobenzene	15	[30]
	n-Pentylbenzene	15	[27]
	Oleic acid	19	[58]
	Oleic acid ethyl ester	5	[58]
	Oleic acid methyl ester	19	[58]
	Palladium (II) acetylacetonate	125	[56]
	p-Dichlorobenzene	14	[51]
	Phenanthrene	25	[24, 38, 59]
	Phenol	110	[37, 42, 43, 54]
	Phenylacetic acid	16	[61]
	Phenylmethanol	15	[28]
	Pyrene	3	[24]
	Stearic acid ethyl ester	34	[44, 45]
	Styrene	15	[25]
	Tetrahydrofuran	15	[57]
	Thenoyltrifluoroacetone	15	[21]
	Toluene	26	[50, 54]
	Triarachidonin	27	[62]
	Trierucin	101	[62]
	Trifluoroacetylacetone	15	[21]
	Trinervonin	38	[62]
	Triolein	10	[58]
	Ubiquinone	71	[63]
	Vanillin	15	[61]
	Liquid systems		
2,2,4-Trimethylpentane	1,3,5-Trimethylbenzene	4	[64]
	Benzene	4	[64]
	Ethylbenzene	4	[64]
	o-Xylene	4	[64]
	p-Xylene	4	[64]
	Toluene	4	[64]
Cyclohexane	Benzene	8	[65]

Table 1: Continued

System		NDP	Data sources
Solvent (1)	**Solute (2)**		
Supercritical systems			
Cyclohexane	Ethane	5	[65]
	Ethylene	5	[65]
	Toluene	4	[66]
n-Decane	12-Crown-4	4	[67]
	15-Crown-5	4	[67]
	18-Crown-6	4	[67]
	Argon	3	[68]
	Carbon tetrachloride	3	[68]
	Dicyclohexano-18-crown-6	4	[67]
	Dicyclohexano-24-crown-8	4	[67]
	Krypton	3	[68]
	Methane	3	[68]
	s-Trioxane	4	[67]
	Tetrabutyltin	4	[68]
	Tetraethyltin	3	[68]
	Tetramethyltin	4	[68]
	Tetrapropyltin	4	[68]
	Xenon	4	[68]
n-Dodecane	1,3,5-Trimethylbenzene	4	[66]
	Acetone	5	[66]
	Benzene	4	[66]
	Carbon dioxide	9	[69]
	Carbon monoxide	9	[69]
	Hydrogen	9	[69]
	Linoleic acid methyl ester	4	[66]
	m-Xylene	4	[66]
	Naphthalene	5	[66]
	n-Decane	5	[70]
	n-Hexadecane	5	[70]
	n-Octane	9	[70]
	n-Tetradecane	5	[70]
	Toluene	4	[66]
n-Eicosane	Carbon dioxide	5	[71]
	Carbon monoxide	5	[71]
	Hydrogen	5	[71]
	n-Dodecane	5	[71]
	n-Hexadecane	5	[71]
	n-Octane	5	[71]
n-Heptane	*n*-Decane	5	[70]
	n-Dodecane	5	[70]
	n-Hexadecane	8	[70]
	n-Octane	4	[70]
	n-Tetradecane	5	[70]
n-Hexadecane	Carbon dioxide	10	[69]
	Carbon monoxide	10	[69]
	Hydrogen	10	[69]
	n-Decane	5	[72]

Table 1: Continued

System		NDP	Data sources
Solvent (1)	**Solute (2)**		
Supercritical systems			
n-Hexadecane	*n*-Dodecane	5	[72]
	n-Octane	10	[72]
	n-Tetradecane	5	[72]
n-Hexane	1,3,5-Trimethylbenzene	20	[66, 73]
	Acetone	5	[66]
	Acetonitrile	7	[74]
	Benzene	39	[64, 66, 73, 74]
	Carbon disulphide	10	[74]
	m-Xylene	5	[66]
	Naphthalene	26	[66, 73, 74]
	Phenanthrene	15	[73]
	p-Xylene	17	[66, 73]
	Toluene	20	[66, 73]
n-Octacosane	Carbon dioxide	5	[75]
	Carbon monoxide	5	[75]
	Hydrogen	5	[75]
	n-Dodecane	5	[75]
	n-Hexadecane	5	[75]
	n-Octane	5	[75]
n-Octane	1,3,5-Trimethylbenzene	4	[64]
	Argon	4	[68]
	Benzene	4	[64]
	Carbon tetrachloride	4	[68]
	Ethylbenzene	4	[64]
	Krypton	4	[68]
	Methane	4	[68]
	o-Xylene	4	[64]
	p-Xylene	4	[64]
	Tetrabutyltin	4	[68]
	Tetraethyltin	5	[68]
	Tetramethyltin	4	[68]
	Tetrapropyltin	4	[68]
	Toluene	4	[64]
	Xenon	4	[68]
	Gas systems		
Argon	Ethane	9	[76]
	Helium	11	[77, 78]
	Hydrogen	5	[77]
	i-Butane	8	[76]
	Methane	9	[76]
	n-Butane	8	[76]
	Neon	11	[77, 79]
	Propane	9	[76]
Carbon dioxide	Helium	7	[80]
	Hydrogen	7	[80]
Carbon monoxide	Helium	7	[80]
	Hydrogen	7	[80]

Table 1: Continued

System		NDP	Data sources
Solvent (1)	**Solute (2)**		
Supercritical systems			
Deuterium	Hydrogen	5	[77]
Ethane	Nitrogen	7	[80]
Ethylene	Nitrogen	7	[80]
Helium	Hydrogen	12	[77, 81]
Krypton	Argon	6	[82]
	Helium	6	[82]
	Neon	12	[80, 82]
	Xenon	9	[82]
Methane	Carbon dioxide	10	[83]
	Tetrachloroethene	5	[84]
Neon	Deuterium	5	[77]
	Helium	24	[77-79]
	Hydrogen	5	[77]
Nitrogen	Ethane	7	[85]
	Methane	7	[85]
	n-Butane	5	[85]
	Propane	6	[85]
Tetrafluoromethane	1,1,1-Trichloroethane	5	[84]
	Tetrachloroethene	5	[84]
Xenon	Neon	6	[79]

Critical properties (critical temperature, critical pressure and critical volume) and molecular descriptors are available in literature [2], which estimated by several equations. In Table 2 variation range of each parameter (input data) and infinite dilute diffusion coefficient (output data) are summarized for SCF, liquid and gas systems.

1.2. Neural network training

After determination of input data, ANN was designed. In this case a three-layer feed forward network has been used. Number of neurons in hidden layer should has a minimum value and if training error of network with these number of neurons does not have expected value, number of neurons is increased one by one to achieve desired value [86]. By applying neural network for infinite dilute diffusion coefficient of SCF, liquid and gas systems and changing number of neurons in hidden layer, number of optimal neurons was found in hidden layer as 21, 19 and 18, respectively (attend to Table 3). In these models, *tansig* transfer function in hidden layer and *purelin* transfer function in output layer were used which are defined as follow:

$$f_{\text{tansig}}(\chi)=\frac{e^{\chi}-e^{-\chi}}{e^{\chi}+e^{-\chi}} \tag{2}$$

$$f_{\text{purelin}}(\chi)=\chi \tag{3}$$

Also output of one neuron is computed by following equation:

$$O_j = f_{\text{purelin}}\left\{\sum_{k=1}^{m} w_{jk}^{OL}\left[f_{\text{tansig}}\left(\sum_{i=1}^{n}\left(w_{ji}^{HL}x_i\right)+b_j^{HL}\right)\right]_k + b_j^{OL}\right\} \tag{4}$$

For training of data, neural network algorithm of LM [87-89] was used. Performance function of this algorithm is MRE ($MRE=(100/NDP)\sum_{i=1}^{NDP}\left|\left(D_{12}^{calc.}-D_{12}^{\exp.}\right)/D_{12}^{\exp.}\right|_i$), maximum number of epochs is 500 and performance goal is 10^{-5}.

Table 2: Variations range of input and output of neural network

Property	Supercritical systems		Liquid systems		Gas systems	
	Minimum	Maximum	Minimum	Maximum	Minimum	Maximum
$M_1(\mathrm{g/mol})$	44.01	86.18	84.16	394.77	4.00	131.30
$T_{c1}(\mathrm{K})$	304.10	500.00	507.50	864.27	5.19	305.40
$P_{c1}(\mathrm{MPa})$	3.13	7.38	0.66	4.07	0.23	7.38
$V_{c1}\left(\mathrm{cm}^3/\mathrm{mol}\right)$	93.90	358.00	308.00	1603.50	41.60	148.30
$T_{bp1}(\mathrm{K})$	194.70	331.10	341.90	704.75	4.25	194.70
$V_{bp1}\left(\mathrm{cm}^3/\mathrm{mol}\right)$	33.28	135.31	115.57	651.26	14.18	53.73
$\sigma_{LJ1}\left(\mathrm{\AA}\right)$	3.58573	5.60165	5.32769	9.23375	2.73350	4.17576
$\{\varepsilon_{LJ}/k_B\}_1(\mathrm{K})$	241.48	397.05	403.00	686.31	4.12	830.49
$M_2(\mathrm{g/mol})$	32.04	1137.91	2.02	460.61	2.02	165.83
$T_{c2}(\mathrm{K})$	412.85	1601.10	33.00	1357.66	5.19	620.20
$P_{c2}(\mathrm{MPa})$	0.25	8.09	1.25	7.90	0.23	7.38
$V_{c2}\left(\mathrm{cm}^3/\mathrm{mol}\right)$	118.00	3081.54	64.30	1210.75	41.60	289.60
$T_{bp2}(\mathrm{K})$	299.15	1229.05	20.30	1077.88	4.25	394.40
$V_{bp2}\left(\mathrm{cm}^3/\mathrm{mol}\right)$	42.28	1291.44	22.38	485.16	14.18	108.35
$\sigma_{LJ2}\left(\mathrm{\AA}\right)$	3.86945	11.48007	3.16052	8.40827	2.73350	5.21941
$\{\varepsilon_{LJ}/k_B\}_2(\mathrm{K})$	4.12	1271.42	26.21	1078.11	4.12	830.49
$T(\mathrm{K})$	288.35	548.20	101.80	567.00	76.60	4262.00
$P(\mathrm{MPa})$	5.35	40.11	0.101	385.600	0.101	0.101
$D_{12}\times10^4\left(\mathrm{cm}^2/\mathrm{s}\right)$	0.28	6.44	0.04	11.80	0.04×10^4	10.80×10^4

2. Results and discussion

Results of determination of the optimal number of neurons in hidden layer for SCF, liquid and gas are presented in Table 3. According to Table 3 the best neural networks for SCF, liquid and gas systems has 21, 19 and 18 neuron in hidden layer, respectively. As it presented in Table 3 MRE of test data for SCF, liquid and gas systems are 3.49, 2.60 and 2.38 %, respectively.

Figure 1 shows a correlation between results of training and test data of neural network and experimental data for SCF. Also in this Figure percent of relative error ($\mathrm{RE}=100\times\left(D_{12}^{calc.}-D_{12}^{\exp.}\right)/D_{12}^{\exp.}$) for each training and test data has been shown. Figures 2 and 3 show the similar results for liquid and gas systems, respectively. As it can be observed from Figures 1 to 3, there exist a good correlation between experimental data and neural network models output.

In this study, estimation of infinite dilute diffusion coefficient by ANN model has been compared with the results of the existed correlations and equations in the literature [2]. Correlations that have been used in literature [2] with their sources were summarized in Table 4. In addition to correlations represented in Table 4, real fluid theory was also used for estimation of infinite dilute diffusion coefficient [2]. Eqs. (5)-(8) for SCF and liquid, and Eq. (10) were used just for SCF, but Eqs. (13) and (21) and real fluid theory (Eq (22)) were used for SCF, liquid and gas.

Table 3: Determining of optimal number of neuron in hidden layer for SCF, liquid and gas systems

	MRE								
	train	test	total	train	test	total	train	test	total
No. of neurons	Supercritical systems			Liquid systems			Gas systems		
9	4.29	4.33	4.30	5.82	5.98	5.86	0.89	5.88	2.14
10	4.02	4.43	4.11	4.92	4.43	4.80	1.08	2.37	1.41
11	3.82	4.37	3.95	3.86	3.43	3.75	0.96	2.71	1.40
12	3.81	4.28	3.92	4.28	4.03	4.21	0.71	11.12	3.31
13	3.30	4.26	3.52	3.81	3.46	3.72	0.96	9.50	3.10
14	3.23	3.76	3.36	4.07	3.54	3.94	0.96	3.78	1.67
15	3.48	4.16	3.64	4.44	4.28	4.40	0.97	4.22	1.78
16	3.19	5.08	3.62	3.16	2.94	3.11	0.84	3.03	1.38
17	3.39	5.80	3.94	3.32	2.66	3.16	0.84	2.67	1.29
18	3.41	3.93	3.53	5.67	5.04	5.51	**0.82**	**2.38**	**1.21**
19	3.09	3.59	3.21	**3.12**	**2.60**	**2.99**	0.95	3.87	1.68
20	3.20	3.65	3.30	3.68	3.58	3.66	0.91	2.79	1.38
21	**2.85**	**3.49**	**3.00**	3.42	2.67	3.23	0.82	4.50	1.74
22	2.91	3.94	3.15	3.19	2.74	3.08	0.73	6.97	2.29
23	2.90	4.52	3.28	3.57	3.04	3.44	0.83	3.37	1.46

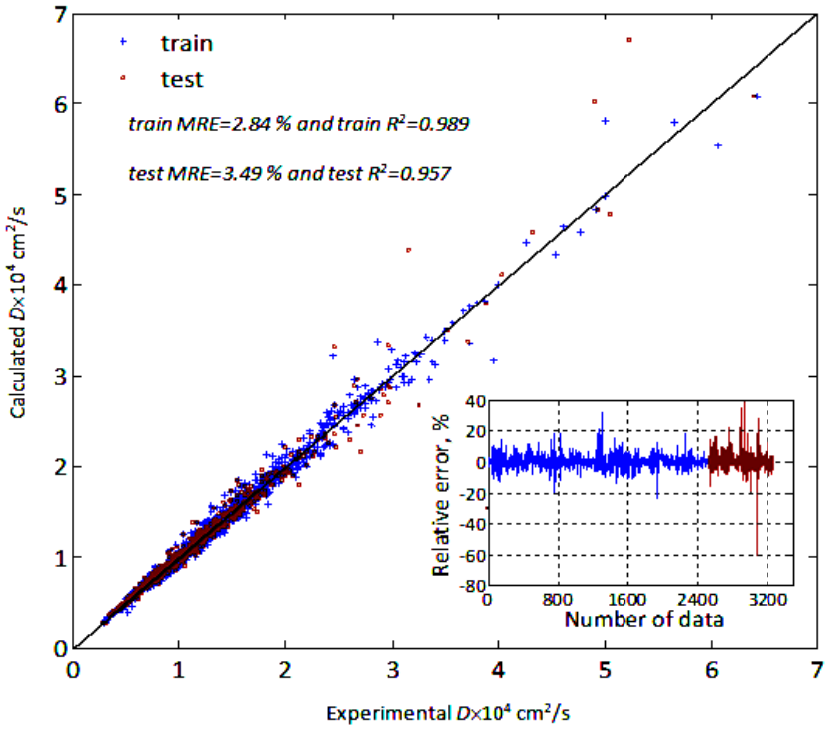

Figure 1: Comparison between calculated and experimental infinite dilute diffusion coefficient for SCF

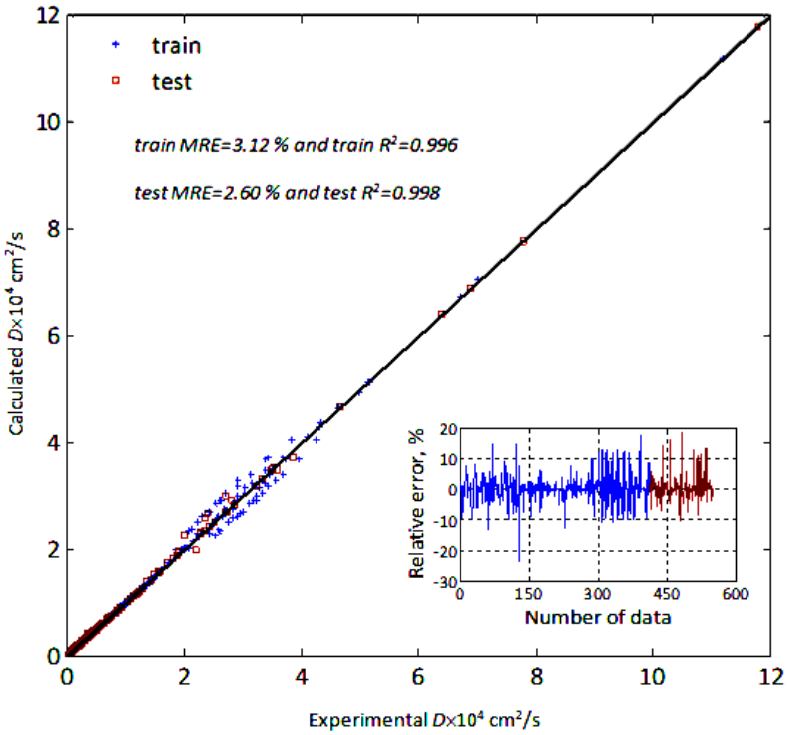

Figure 2: Comparison between calculated and experimental infinite dilute diffusion coefficient for liquid

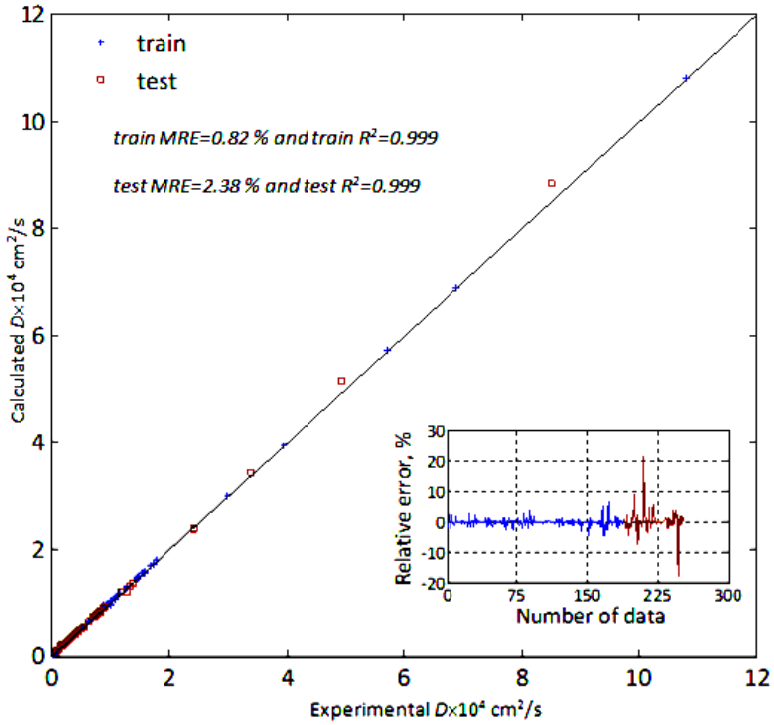

Figure 3: Comparison between calculated and experimental infinite dilute diffusion coefficient for gas

Table 4: Correlations and equations for infinite dilution diffusion coefficients

Equations and correlations	Infinite dilution diffusion coefficients	
Wilke-Chang equation [1, 90, 91]	$D_{12} = 7.4\times10^{-8}\dfrac{T\sqrt{\Phi M_1}}{\eta_1 V_{bp,2}^{0.6}}$	(5)
	for CO_2 $\Phi = 1$	
Tyn-Calus equation [1, 92]	$D_{12} = 8.93\times10^{-8}\dfrac{V_{bp,1}^{0.267}}{V_{bp,2}^{0.488}}\dfrac{T}{\eta_1}$	(6)
	this equation is for most organic solvents	
Scheibel equation [1, 93]	$D_{12}=\dfrac{8.2\times10^{-8}T}{\eta_1 V_{bp,3}^{1/3}}\left[1+\left(\dfrac{3V_{bp,1}}{V_{bp,2}}\right)^{2/3}\right]$	(7)
Reddy-Doraiswamy equation [1, 94]	$D_{12} = \beta\times\dfrac{T\sqrt{M_1}}{\eta_1\left(V_{bp,1}V_{bp,2}\right)^{1/3}}$	(8)
	If $\dfrac{V_{bp,1}}{V_{bp,2}}\le1.5\Rightarrow\beta=10\times10^{-8}$ and $\dfrac{V_{bp,1}}{V_{bp,2}}>1.5\Rightarrow\beta=8.5\times10^{-8}$	(9)
He-Yu-Su correlation [95]	$D_{12} = \dfrac{A\times10^{-7}\left(V_1^k - B\right)T}{\sqrt{M_2}}$	(10)
	If $\rho_{r,1}\ge1.2\Rightarrow k=1$ and $\rho_{r,1}<1.2\Rightarrow k=1+\dfrac{\left(\rho_{r,1}-1.2\right)}{\sqrt{M_1}}$	(11)
	$A = 0.29263 + 1.6736e^{\left(-\frac{0.75832\sqrt{M_1V_{c,1}}}{P_{c,1}}\right)}$ and $B = 0.077T_{c,1}$	(12)
Model of Zhu el al. [96]	$D_{12} = \dfrac{3}{8\sqrt{\pi}}\sqrt{\dfrac{\sigma_{12,LJ}^2\varepsilon_{12,LJ}}{m_1}\dfrac{\sqrt{T_{12}^*}}{\rho_{12}^*}}\left(1-\dfrac{\rho_{12}^*}{1.029079T_{12}^{*\,0.165877}}\right)\times$ $\left[1+\rho_{12}^{*\,0.126978}\left(\dfrac{0.596103\left(\rho_{12}^*-1\right)}{0.539292\left(\rho_{12}^*-1\right)+T_{12}^{*\left(0.400152-0.41054\rho_{12}^*\right)}}+0.68856\right)\right]\times e^{\left(\frac{\rho_{12}^*}{2T_{12}^*}\right)}$	(13)
	$T_{12}^* = \dfrac{T}{\varepsilon_{12,LJ}/k_B}$, $\rho_{12}^* = \rho_1\sigma_{12}^3$	(14)
	$\dfrac{\varepsilon_{12,LJ}}{k_B} = \sqrt{\dfrac{\varepsilon_{1,LJ}}{k_B}\times\dfrac{\varepsilon_{2,LJ}}{k_B}}$	(15)
	$\sigma_{12,LJ} = \left(1-k_{12}^d\right)\dfrac{\sigma_{1,LJ}+\sigma_{2,LJ}}{2}$ where $k_{12}^d = 0.7926\dfrac{\sigma_{2,LJ}-\sigma_{1,LJ}}{\sigma_{1,LJ}+\sigma_{2,LJ}}$	(16)
	$\dfrac{\varepsilon_{1,LJ}}{k_B} = \dfrac{T_{c,1}}{T_{c,1}^*}\left[1+0.47527332\rho_{r,1}+\left(0.06300484+0.12374707\rho_{r,1}\right)T_{r,1}\right]$	(17)
	$\sigma_{1,LJ} = \left(\dfrac{\rho_{c,1}^*}{\rho_{c,1}}\right)^{1/2}\left[1-0.368868\rho_{r,1}+\left(0.0000694+0.01089228\rho_{r,1}\right)T_{r,1}\right]$	(18)
	$\dfrac{\varepsilon_{2,LJ}}{k_B} = \dfrac{T_{c,2}}{1.313}$	(19)
	$\sigma_{2,LJ} = \sqrt[3]{\dfrac{0.13\varepsilon_{2,LJ}}{P_{c,2}}}$	(20)

Table 4: Continued

Equations and correlations	Infinite dilution diffusion coefficients	
Dymond-Hildebrand-Batschinski free-volume expression [97, 98, 99]	$D_{12} = B\sqrt{T}\left(V_1 - V_D\right)$	(21)
Real fluid theory [2]	$D_{12,LJ} = \dfrac{k_B T}{\xi_{12,R} + \xi_{12,S}}$	(22)
	$\xi_{12,R} = \dfrac{8}{3}\rho_1 \sigma_{12,eff}^2 \sqrt{2\pi m_{12} k_B T}\, \dfrac{g\left(\sigma_{12,eff}\right)}{F_{12}}$	(23)
	$\xi_{12,S} = \dfrac{8}{3}\rho_1 \sigma_{12,eff}^2 \sqrt{2\pi m_{12} k_B T}\, \dfrac{0.4}{T_{12}^{*\,1.5}}$	(24)
	$\sigma_{12,eff} = 1.1532\sigma_{12,LJ}\left[1 + \left(1.8975 T_{12}^*\right)^{1/2}\right]^{-1/6}$	(25)

Table 5: Mean relative error for SCF, liquid and gas systems

System	NDP[a]	NDP[b]	NS[a]	NS[b]	ANN MRE	Eq. (22)	Eq. (21)	Eq. (13)	Eq. (10)	Eq. (5)	Eq. (6)	Eq. (7)	Eq. (8)
Supercritical	3277	3297	111	111	3.00	4.16	4.02	40.34	7.84	12.77	15.93	16.71	76.16
Liquid	549	548	88	87	2.99	5.66	5.83	38.56	-	43.85	44.19	80.98	45.39
Gas	252	251	32	28	1.21	1.83	2.01	43.30	-	-	-	-	-
Total	4078	4096	231	226	2.88	4.22	4.14	40.28	7.83	17.20	19.96	25.87	71.77

[a] NDP and NS for ANN model.
[b] NDP and NS for literature [2].

The minimum and maximum relative errors by ANN are 0.1 % (*n*-Octacosane-Carbon dioxide liquid system and Carbon monoxide-Helium gas system) and 9.73 % (Carbon dioxide-Acridine SCF system). Number of data of carbon dioxide-Acridine system are 6 which in comparison with other supercritical systems is a low value. So probability of using these data by ANN comes down and for estimating of infinite dilute diffusion coefficient, ANN model utilizes other substances data that have similar properties to Acridine and this subject caused low accuracy estimation. Also total results are available in Table 5. As shown in this table the MRE for ANN in SCF, liquid and gas systems is 3.00, 2.99 and 1.21 %, respectively and average of total error is 2.88 %.Total relative error for Eqs. (5)-(8) are changed from 17.2 to 71.77 % (see Table 5). Eq. (10) that is used just for SCF has a MRE=7.83 %, and Eq. (13) has a poor results (MRE=40.28 %). Eqs. (22) (Real fluid theory) and (21) have a remarkable accuracy and MRE of 4.22 and 4.18 %, respectively.

3. Conclusions

In this work, artificial neural network models were investigated for estimation of infinite dilute diffusion coefficient of binary SCF (111 systems/3277 points), liquid (88 systems/549 points) and gas (32 systems/252 points) systems. For each one of SCF, liquid and gas systems a three-layer feed forward neural network with train algorithm of LM was used. In hidden and output layers, transfer function of 'tansig' and 'purelin' were used, respectively. By applying each one of the networks on three-fourths of data, optimal number of neurons in hidden layer for SCF, liquid and gas systems is 21, 19 and 18, respectively. Calculation results are shown high accuracy of neural network models for SCF, liquid and gas systems by MRE equal to 3.00, 2.99 and 1.21 %, respectively.

Nomenclature

A	parameter in Eq. (10)
B	parameter in Eqs. (10) and (21)
b_j	bias of j th neuron
D	tracer diffusion coefficient, cm^2/s
F	correction factor in Eq. (23)

f transfer function
$g(\sigma)$ radial distribution function at contact
k parameter in Eq. (10)
k_{12} binary interaction parameter
k_{12}^{d} interaction parameter in Eq. (15)
k_B Boltzmann constant, 1.380658×10^{-16} g.cm^2 / s^{2}K
M molecular weight, g/mol
m mass of a molecule, g
NS number of systems
O_j output of j th neuron
P pressure, MPa
T temperature, K
V molar volume, cm^3 / mol
V_D parameter in Eq. (21), cm^3 / mol
w_{ji} synaptic weight corresponding to i th synapse j th neuron
w_{jk} synaptic weight corresponding to k th synapse j th neuron
x_i i th input signal to j th neuron

Greek letters

β parameter in Eq. (8)
χ input value of neural network
ε / k_B Lennard–Jones energy parameter, K
Φ dimensionless association factor of the solvent
η viscosity, cP
ρ density number, cm^{-1}
σ molecular diameter, cm
ξ friction coefficient

Subscripts

1 solvent
2 solute
12 binary property
bp boiling point
c critical property
eff effective hard sphere diameter
LJ Lennard–Jones fluid
R repulsive contribution
r reduced property
S soft attractive contribution

Superscripts

$*$ reduced quantity
HL hidden layer
OL output layer

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